LETTER TO THE EDITOR

Coarsening in surface growth models without slope selection♯

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Abstract. We study conserved models of crystal growth in one dimension [$\partial_t z(x,t) = -\partial_x j(x,t)$] which are linearly unstable and develop a mound structure whose typical size L increases in time ($L \sim t^n$). If the local slope ($m = \partial_x z$) increases indefinitely, n depends on the exponent γ characterizing the large m behaviour of the surface current j ($j \sim 1/|m|^\gamma$): $n = 1/4$ for $1 \leq \gamma \leq 3$ and $n = (1+\gamma)/(1+5\gamma)$ for $\gamma > 3$.

The conserved dynamics of a solid surface growing under the action of an external flux of particles is described by the continuum equation

$$\partial_t z(x,t) = -\partial_x j(x,t) + \delta F(x,t) \ , \tag{1}$$

where $z(x,t)$ is the local height of the surface in a comoving frame (so that the average value $\bar{z}$ is set to 0) and $\delta F(x,t)$ is the shot noise.

Thermodynamic and kinetic mechanisms contribute to j and its actual expression depends on the details of the growth process. Here we are interested in the growth of a high-symmetry surface by Molecular Beam Epitaxy (MBE), where the instability has a purely kinetic origin: the reduced interlayer diffusion [1]. Nonetheless, our treatment will be as general as possible.

A wide class of models is described by the current

$$j = K m''(x) + j_{\rm ES}(m) \ , \tag{2}$$

where $m = \partial_x z$ is the local slope. The first term generally describes a thermally activated relaxation of the surface, but kinetic mechanisms can also contribute to K [2].

The second term is responsible for the instability and its origin is an asymmetry in the sticking process of an adatom to a step (Ehrlich-Schwoebel (ES) effect): sticking from the upper terrace is hindered and this implies an up-hill current [3] which is called Ehrlich-Schwoebel current ($j_{\rm ES}$). Also other (generally stabilizing) processes can contribute to $j_{\rm ES}$ and this explains the different expressions $j_{\rm ES}$ may take [4].

♯ Dedicated to the Peanuts on the occasion of their 50th birthday.

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Whatever these processes are, $j_{\rm ES}$ is linear in m at small slopes ($j_{\rm ES} \sim \nu m$) and therefore in the early stages of the growth it prevails on the first term (Km'') at sufficiently large wavelengths. This means that the linear stability of the flat surface will be decided by the sign of ν, a positive one meaning instability. In fact, in the limit $m \to 0$ we have

$$\partial_t z = -K\partial_x^4 z - \nu\partial_x^2 z \tag{3}$$

whose solution is $z(x,t) = \exp(\omega_q t)\cos(qx)$ with $\omega_q = \nu q^2 - Kq^4$. An up-hill current means that $j_{\rm ES}$ has the same sign as the slope, so ν is positive and the flat surface is unstable ($\omega_q > 0$) against modulations of wavevector smaller than $\bar{q} = \sqrt{\nu/K}$; the instability appears after a typical time of order $t^* \simeq (\nu\bar{q}^2)^{-1} = K/\nu^2$.

The later evolution of the surface depends on the nonlinear form of the unstable current $j_{\rm ES}(m)$. By taking the spatial derivative of Eq. (1), we obtain

$$\partial_t m = \partial_x^2(-j) + \partial_x(\delta F) \tag{4}$$

and a parallel with a phase ordering process is easily done, once we remark that the current can be obtained by a pseudo free energy $\mathcal{F}$:

$$j = -\frac{\delta\mathcal{F}}{\delta m}\,, \quad \mathcal{F}[m] = \int {\rm d}x \left[\frac{K}{2}(\partial_x m)^2 + V(m)\right]\,, \quad V'(m) = -j_{\rm ES}(m)\,. \tag{5}$$

The instability of the flat surface ($j'_{\rm ES}(0) > 0$) means that the potential $V(m)$ has a maximum in $m = 0$ ($V''(0) < 0$). Contiguous regions of increasing and opposite slope are formed. The usual phase ordering process is obtained when $V(m)$ has the classical double well form: $V(m) = -(\nu/2)m^2 + (\nu/4m_0^2)m^4$, corresponding to a current $j_{\rm ES} = \nu m(1 - m^2/m_0^2)$. After the slope has attained a fraction of m_0 the dynamics enters in the nonlinear regime: the wavelength L of the profile increases in time (coarsening process) and the slope saturates to the constant values $\pm m_0$. The coarsening law is known to be logarithmic [5] ($L(t) \sim \ln t$) in absence of shot noise and a power law [6] ($L(t) \sim t^{1/3}$), in presence of it.

The aim of the present paper is to analyze the *deterministic* ($\delta F(x,t) \equiv 0$) growth process when $V(m)$ has no minima, corresponding to the absence of zeros at finite slopes in the current $j_{\rm ES}$. We will consider the class of currents defined by

$$j_{\rm ES} = \frac{\nu m}{(1 + \ell^2 m^2)^\alpha} \qquad \text{with} \quad \alpha \geq 1 \tag{6}$$

and the corresponding models will be termed α-models.

Model-1 has been studied numerically by Hunt *et al* [7] and they found a coarsening exponent $n \approx 0.22$ ($L(t) \sim t^n$). α-Models without noise have been studied analytically by Golubović [8] through scaling arguments and he finds $n = 1/4$ irrespectively of α. Finally, qualitative considerations based on noise effects [9] give $n = 1/(2/\alpha + 3)$, i.e. $n = 1/5$ for model-1.

Our analytical approach is based on the linear stability analysis of the stationary configurations $j[m(x)] \equiv 0$. This way, the finding of the coarsening exponent n passes through the determination of the lowest eigenvalue of the operator $(-\partial_x^2)\hat{H}$, where $\hat{H}$ is the Hamiltonian corresponding to a particle in a periodic potential [5].

Before proceeding we render adimensional the growth equation by rescaling x with $1/\bar{q}$, t with t^* and z with $1/\bar{q}\ell$:

$$\partial_t z = -\partial_x j \ , \qquad j = m'' + \frac{m}{(1+m^2)^\alpha} \ . \tag{7}$$

Stationary configurations are the solutions of the differential equation $j[m(x)] = m'' + j_{\rm ES}(m) \equiv 0$. Therefore they correspond to the periodic orbits of a particle in the potential $-V(m) = -[1/2(\alpha-1)](1+m^2)^{1-\alpha}$ for $\alpha > 1$ and in the potential $-V(m) = (1/2)\ln(1+m^2)$ for $\alpha = 1$. In the former case the potential is upper bounded and the solution corresponding to the boundary conditions $m \to \pm\infty$ when $x \to \pm\infty$ does exist, while it does *not* for $\alpha = 1$ because the corresponding energy would be infinite. Stationary solutions may be labelled with their period, i.e. the wavelength L: $m_L(x)$.

Let us now perform a linear stability analysis around these stationary and periodic solutions: $m(x,t) = m_L(x) + \psi(x,t)$. It is easily found that

$$\partial_t \psi = \partial_x^2 \left[-\psi''(x,t) + U_L(x)\psi\right] \ , \tag{8}$$

where $U_L(x) \equiv -j'_{\rm ES}(m_L(x))$. By putting $\psi(x,t) = \phi(x)\exp(-\epsilon t)$ we obtain

$$(-\partial_x^2)\left[-\phi''(x) + U_L(x)\phi\right] \equiv D_x \hat{H}\phi(x) = \epsilon\phi \ . \tag{9}$$

Negative eigenvalues mean that $m_L(x)$ is linearly unstable and this induces the coarsening process; moreover, $\epsilon(L) \to 0^-$ when $L \to \infty$. The dependence of the ground state (GS) energy on the distance L determines the time scale of the coarsening process: $t \sim 1/|\epsilon(L)|$. For the moment we will assume $D_x \equiv 1$, i.e. we will consider the *nonconserved* model: $\partial_t m = -\delta\mathcal{F}/\delta m$.

First of all we observe that in the limit of large L the energy shift $\epsilon(L)$ for the periodic potential is equal (up to a numerical factor) to the shift for a single couple of potential wells [10]. The solution of the problem is given [11] in terms of ϕ_0 and ϕ_1, respectively the ground state for the single well $U_1(x)$, centered in $x = L$, and for the double well $U_2(x)$, centered in $x = \pm L$. In fact the Schroedinger equations are:

$$-\phi_0'' + U_1\phi_0 = 0 \quad (a) \qquad\qquad -\phi_1'' + U_2\phi_1 = \epsilon\phi_1 \quad (b) \tag{10}$$

and by evaluating the quantity $\int_0^\infty {\rm d}x[\phi_1 \times (10a) - \phi_0 \times (10b)] = 0$, we obtain

$$\phi_1(0)\phi_0'(0) = -\epsilon \int_0^\infty {\rm d}x \phi_0(x)\phi_1(x) \ , \tag{11}$$

where we have made use of $U_1 = U_2$ for $x > 0$.

Before proceeding we must determine the asymptotic expressions of $\phi_0(x)$ and $\phi_1(x)$. The potential $U(x) = -j'_{\rm ES}(m)$ is given, for α-models, by

$$U(x) = \frac{(2\alpha-1)m^2 - 1}{(1+m^2)^{\alpha+1}} \to \frac{(2\alpha-1)}{m^{2\alpha}} \ . \tag{12}$$

The asymptotic behaviour of the single-mound profile is obtained by integrating the equation $m''(x) + j_{\rm ES}(m) = 0$ and taking the limit $x \to \infty$:

$$(1/2)(m')^2 - V(m) = 0 \quad \Rightarrow \quad \frac{dm}{dx} \approx \frac{1}{\sqrt{\alpha-1}} \frac{1}{|m|^{\alpha-1}} \ . \tag{13}$$

The result $m^\alpha(x) \approx (\alpha/\sqrt{\alpha-1})x$, when inserted in (12) gives:

$$U(x) \approx \frac{(2\alpha-1)(\alpha-1)}{\alpha^2}\frac{1}{x^2} \equiv \frac{a}{x^2} \ , \tag{14}$$

with a increasing between $a=0$ (for $\alpha=1$) and $a=2$ (for $\alpha=\infty$).

The solution of the Schroedinger equation (10a) for $U_1(x) \approx a/(x-L)^2$ gives a *power-law* decaying wavefunction ($\phi_0(x) \sim |x-L|^{-\beta}$), with an exponent $\beta = (1-1/\alpha)$.

If $\alpha \leq 2$ then $\beta \leq 1/2$ and therefore the GS $\phi_0(x)$ of the single well is not a bound state, since $\int_{-\infty}^{\infty} \mathrm{d}x \phi_0^2(x) = \infty$. On the other hand, for $\alpha > 2$ $\phi_0(x)$ is a bound state and $\phi_1(x)$ can be approximated [11] with the expression $\phi_1(x) = [\phi_0(x) + \phi_0(-x)]/\sqrt{2}$. This way, from (11) we easily obtain the relation

$$\epsilon \simeq -2\phi_0(0)\phi_0'(0) \approx -L^{-(2\beta+1)} \quad [\alpha > 2 \text{ and } D_x = 1] \ . \tag{15}$$

If $\alpha < 2$, we can put $\phi_1(x) = [\tilde{\phi}_0(x) + \tilde{\phi}_0(-x)]/\sqrt{2}$ where $\tilde{\phi}_0$ is a generalization of ϕ_0 to a negative eigenvalue: $-\tilde{\phi}_0''(x) + (a/x^2)\tilde{\phi}_0(x) = \epsilon\tilde{\phi}_0(x)$. In fact, even if ϕ_0 is not a bound state, ϕ_1 is bounded, because the GS energy ϵ is strictly lower than $U_2(\pm\infty) = 0$. The previous expression for ϕ_1 may be used even if ϕ_0 itself is bounded (i.e. for $\alpha > 2$) and the result for the coarsening exponent does not change.

The asymptotic expression for $\tilde{\phi}_0$ is $\tilde{\phi}_0(x) = \sqrt{x}K_\mu(\sqrt{|\epsilon|}x)$ where K_μ is the modified Bessel function of order $\mu = \beta - (1/2)$. The function $\tilde{\phi}_0$ decays as a power-law ($\tilde{\phi}_0(x) \approx |\epsilon|^{-\beta/2-1/4}x^{-\beta}$) if $a/x^2 \gg |\epsilon|$ and exponentially ($\tilde{\phi}_0(x) \approx |\epsilon|^{-1/4}\exp(-\sqrt{|\epsilon|}x)$) in the opposite limit, $a/x^2 \ll |\epsilon|$. Eq. (11) now writes

$$\epsilon \int_0^\infty \mathrm{d}x \phi_0(x)\tilde{\phi}_0(x) = -2\tilde{\phi}_0(0)\phi_0'(0) \quad [\alpha \leq 2 \text{ and } D_x = 1] \ , \tag{16}$$

where $\tilde{\phi}_0(x)$ depends on ϵ. Let us remark that the integral I on the left hand side does converge even if ϕ_0 is not a bound state.

The evaluation of the two sides of Eq. (16) is a bit lengthy and we report here the result only: $|\epsilon|\ln(1/|\epsilon|) \sim 1/L^2$ if $\alpha = 2$ and $|\epsilon| \sim 1/L^2$ if $1 < \alpha < 2$. In Fig. 1 we compare the analytical results for the exponent characterizing the energy shift $|\epsilon(L)| \sim L^{-1/n}$ with those obtained through its direct numerical evaluation [12] and the agreement is very good.

Therefore, for the nonconserved model we can conlude that:

$$[\texttt{nonconserved}] \quad n = \frac{1}{2} \ \ (1 < \alpha \leq 2) \quad \text{and} \quad n = \frac{1}{3-2/\alpha} \ \ (\alpha > 2), \tag{17}$$

with a logarithmic correction for $\alpha = 2$ ($L \sim (t/\ln t)^{1/2}$).

The reason why the coarsening exponent n keeps constant for $\alpha < 2$ is the following: if $\alpha > 2$ the single-well wavefunction is a bound state, the integral I is a constant while the 'superposition' between $\phi_0(x)$ and $\phi_0(-x)$ (that is to say the right-hand side of (16)) decreases at increasing α, which implies a decreasing n. Conversely, when $\alpha < 2$ the integral I becomes $\alpha-$dependent and decreases with α: these dependence counterbalances the reduction of the right-hand side of (16).

For the *conserved* growth model, $D_x = -\partial_x^2$ and Eq. (11) must be replaced by a more complicated expression. It has not been possible to carry out a rigorous calculation

because $[\phi_1 \times D_x\hat{H}\phi_0 - \phi_0 \times D_x\hat{H}\phi_1]$ is no more integrable. Nonetheless, there are strong indications that the right-hand sides of (15,16) acquire a factor L^{-2}: the origin of this scaling factor is that $\phi_0(x)$ has a power-like behaviour (and therefore derivation corresponds to divide by x) and also that $U(x) \sim x^{-2}$. Furthermore, since we need the single well wavefunction, corresponding to a zero energy, a solution of the Schroedinger equation $\hat{H}\phi(x) = 0$ is also solution of $D_x\hat{H}\phi(x) = 0$.

As a consequence of such factor, the coarsening exponent for the conserved case is easily obtained from the nonconserved one: $(1/n) \to [(1/n) + 2]$. Therefore:

$$[\texttt{conserved}] \quad n = \frac{1}{4} \quad (1 < \alpha \leq 2) \quad \text{and} \quad n = \frac{1}{5 - 2/\alpha} \quad (\alpha > 2) \; . \quad (18)$$

In order to check numerically the validity of the results reported in Eq.(18) and therefore the dependence of the coarsening exponent n on the parameter α, detailed numerical simulations have been performed. In particular, we have numerically integrated equation (7) by employing a pseudo-spectral time splitting code [13].

The values of $L(t)$, whose log-log plot gives the exponent n, are evaluated through the power spectrum (PS) of $z(x,t)$: the weighted average of the wavevectors corresponding to the most relevant components of the PS is $2\pi/L(t)$. A different method using the spatial correlation function gives consistent results. In Fig. 2, the numerical findings for $n(\alpha)$ by direct integration of Eq. (7) are shown together with the theoretical expression (18) and a good agreement is found.

In conclusion we have found the analytic expression for the coarsening exponents $n(\alpha)$, both for the nonconserved model, Eq. (17) and for the conserved one (growth model), Eq. (18). Coarsening varies with α and it is not logarithmic (i.e. $n = 0$) even for $\alpha = \infty$.

Acknowledgments

We have benefitted a lot by useful discussions with several colleagues: A. Crisanti, C. Godreche, J. Krug, M. Moraldi, W. Strunz and S. Taddei. PP gratefully acknowledges financial support from Alexander von Humboldt Fondation.

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[10] If ϵ_2 is the energy shift for a couple of wells, the shift ϵ_n for n wells is $\epsilon_n = 2\epsilon_2(1 - 1/n)$.

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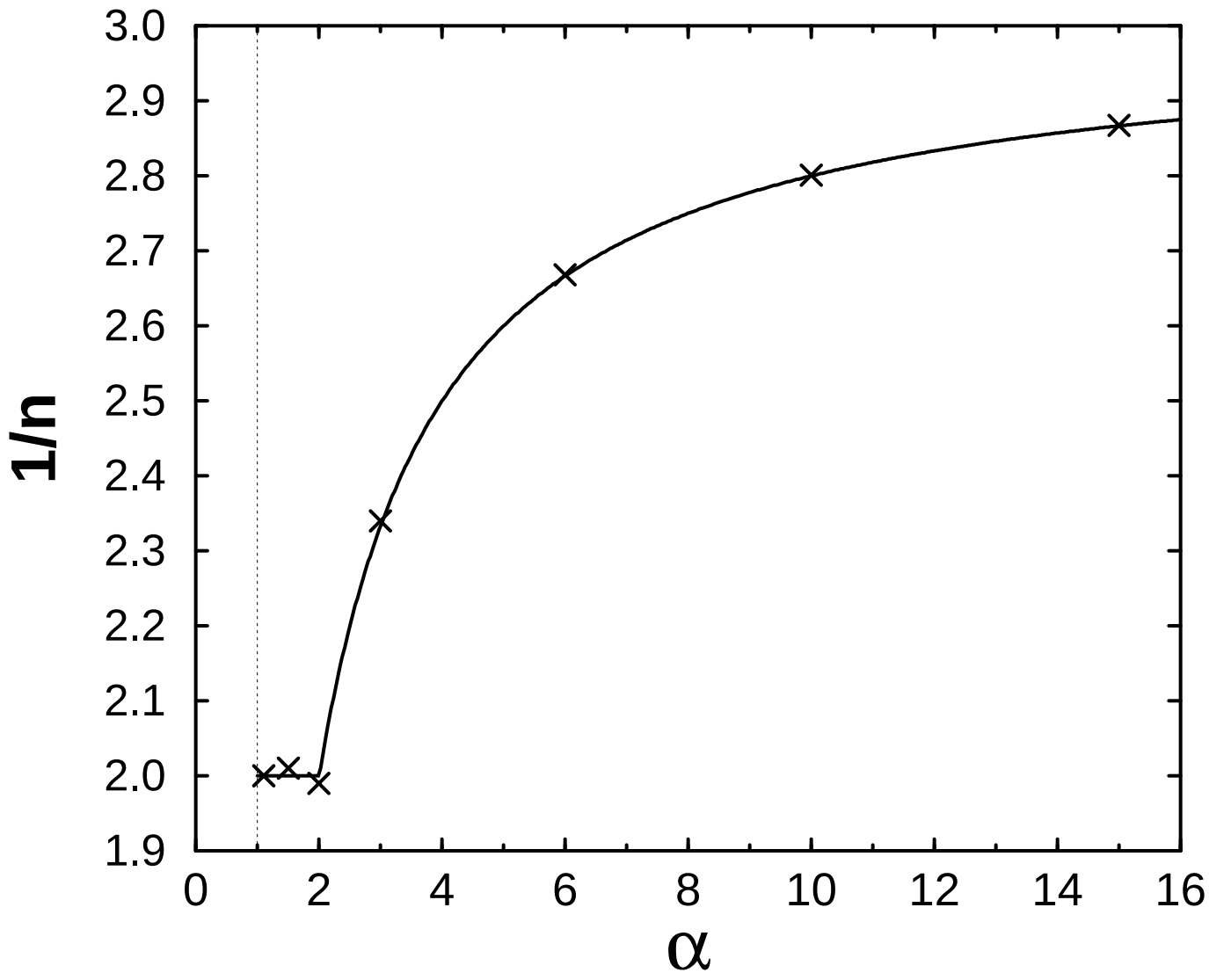
[12] We have considered the single well potential $U(x) = -E_0$ for $|x| < 1$ and $U(x) = a/x^2$ for $|x| > 1$, where $E_0(a)$ is chosen so as to provide a zero GS energy. Afterwards the energy ϵ_2 of the double well problem may be determined by joining the solutions of the Schroedinger equation in each separate "piece" of the potential $U_2(x)$.

[13] The algorithm here employed is analogous to the leap-frog scheme introduced in: Goldmann D and Sirovich L 1995 *Quart. Apll. Math.* **53** 315, for the integration of the complex Ginzburg-Landau equation (CGLE). Here the integration of the nonlinear term cannot be treated analytically as for the CGLE, so we resort to a second order Adams-Bashford scheme. A detailed discussion of this type of algorithms can be found in: Nitti M, Torcini A and Ruffo S 1999 *Int. J. Mod. Phys. C* **10** 1039

Figure captions

Figure 1. Analytical (full line) and numerical (crosses) values for the exponent $1/n$ governing the asymptotic energy shift $|\epsilon_2| \sim 1/L^{1/n}$ (nonconserved model).

Figure 2. Coarsening exponent n for the conserved model. In the inset we enlarge the small α region. Full line is the analytical result (Eq. 18). Points are the exponents found integrating numerically Eq. 7 for a system size $M = 1024$ (spatial resolution $\Delta x = 0.25$) and a total time $400,000 < T < 1,600,000$ (time step $\Delta t = 0.05$). A few tests have also been done with a smaller time step ($\Delta t = 0.025$) and longer chains ($M = 2048$-4096), obtaining consistent results. Bars indicate the numerical fit errors.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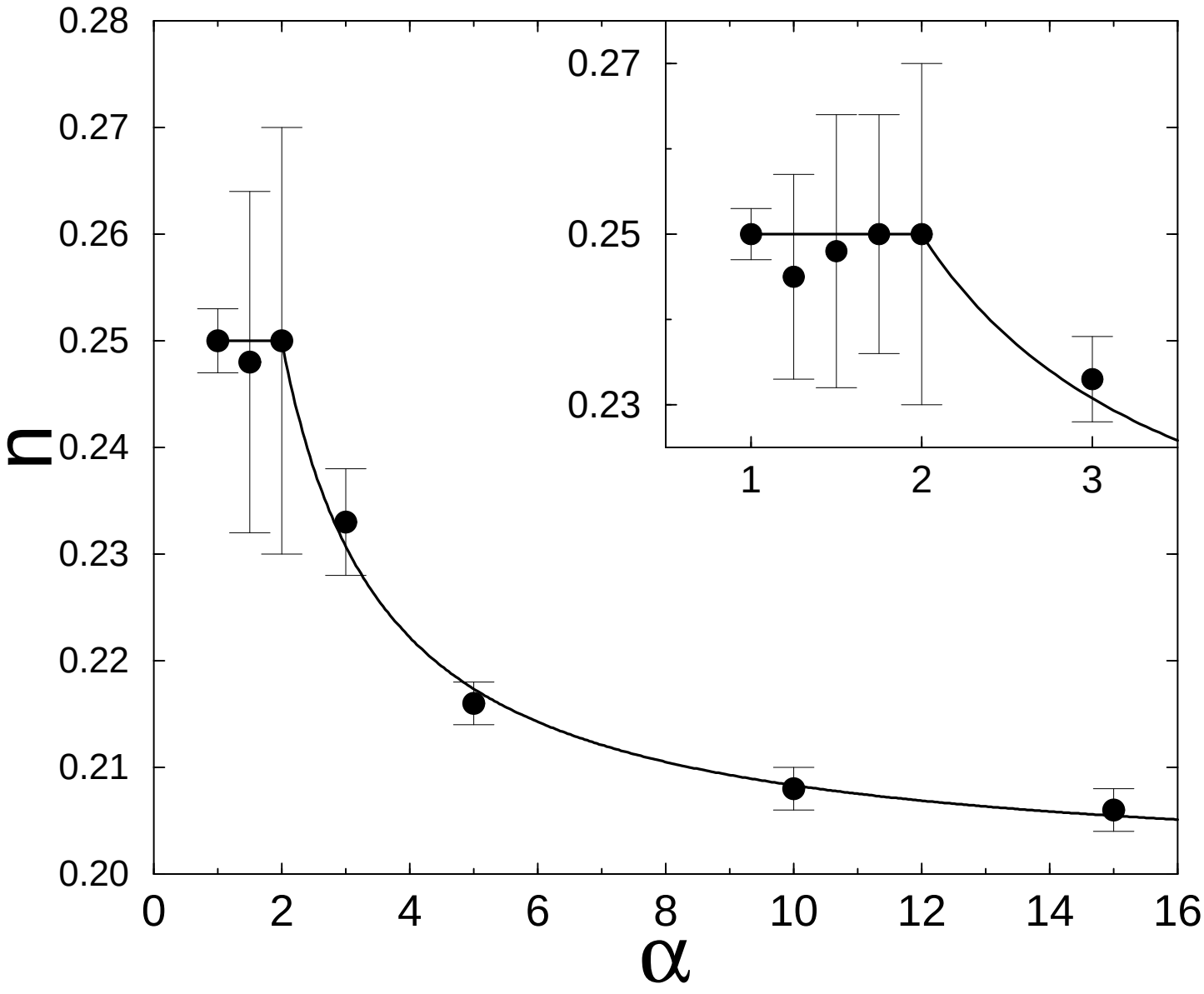
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